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INTRODUCTION

Youngs describes the development of the Rayleigh-Taylor instability in terms of three stages: stage 1, the linear growth phase; stage 2, an interval where the development is nonlinear but predictable from computation given the initial conditions; and stage 3, where all memory of the initial conditions is lost and the flow becomes turbulent.[1] The time interval that stage 2 can be predicted is finite because no matter how accurate the computational method and computer, the accuracy with which the initial conditions can be specified is limited by the experimental noise level and the surface roughness. Although not turbulent, stage 2 very much resembles chaotic motion because what happens in any given run depends sensitively on the initial conditions. There is a new body of theory for treating similar kinds of nonlinear evolution problems and some recent developments in methods for computing Lyapunov exponents may offer a way to describe the stage 2 phase in quantitative statistical terms. Using these methods one can estimate how long the evolution can be predicted given an infinitely accurate computation but some uncertainty in the initial conditions.

Lyapunov exponents measure the average rate at which trajectories in phase space diverge or converge. In a chaotic system the largest Lyapunov exponent tells how fast information is created in bits/sec, and how fast, on average, two solutions with slightly different initial conditions diverge with time. Wolf et al. have recently worked out a way to compute Lyapunov exponents from experimental or computer model generated time series.[2] To get the largest Lyapunov exponent λ_1 they move along the trajectory for a reference solution and compute the quantity,

$$\lambda_1 = 1/(t_m - t_o) \sum_i^m \log_2 [L'(t_i)/L(t_{i-1})] \qquad (1)$$

where $L(t)$ is the distance between solution i and the reference

solution. They pick a point on the reference trajectory, perturb it a little bit, compute L(t), and use that as a starting point for a new solution. They move along this new solution over a short time interval, then stop and compute L(t+Δt). Whenever the new solution begins to diverge too far from the reference solution they stop the calculation, and move back toward the reference trajectory along the line between the two solutions. They keep repeating this process until eventually they have moved over the whole of phase space covered by the reference trajectory. The average rate of divergence converges to λ_1.

Lyapunov exponents are not local quantities; they give the average rate over all of the phase space covered by the given chaotic nonlinear system. But one can use them to get a good estimate for how long one can predict an individual trajectory given a small uncertainty in the initial conditions. Suppose, for example, the initial conditions are specified to 1 part in 1024, ie., with 10 bits of accuracy, and that $\lambda_1 = 2$ bits/s, then we can only predict the future trajectory for a time interval $t = 10 / 2 = 5$ sec.

It may be possible to apply similar ideas to the Rayleigh-Taylor instability evolution to compute a quantity like a largest Lyapunov exponent. In experiments the initial conditions are not known exactly; we only have, at best, a statistical description of the roughness of the interface, but we need to estimate the evolution nevertheless. Every slightly different initial configuration for the interface is going to lead to a much different final configuration. In fact, numerical experimentation shows that each possible solution for some small random initial perturbation of the interface tends to diverge exponentially from every other solution, ie., in Lagrange hydrodynamic computations the mesh configurations diverge. In this context the average we would be interested in would be over the range of all possible final configurations that could evolve starting from a

neighborhood of uncertainty about the initial position. If over this space we had an estimate for a quantity like the largest Lyapunov exponent, then given a parameter describing the roughness, and the largest Lyapunov exponent we would be able to determine how far the interface motion could be computed, and on a more practical level how far in time a layer of material might be expected to stay a layer before becoming a turbulent mix of the adjacent materials.

COMPUTATIONS

One measure of how far apart two solutions are is the rms difference in the position of the lagrange coordinates defining the interface or layer,

$$L_{ij}(t) = \sqrt{\left[\Sigma_n^N \left\{ (x_i(n,t)-x_j(n,t))^2 + (y_i(n,t)-y_j(n,t))^2 \right\} \right]} \qquad (2)$$

where $x_i(n,t)$ and $y_i(n,t)$ are the coordinates of the n^{th} lagrange point of the i^{th} solution at time t, and N is the total number of lagrange points in each solution.

With the above definition for the distance between any two solutions i and j, we can compute a quantity like the largest Lyapunov exponent from,

$$\lambda_1 = (1/m\Delta t) \Sigma_{ij}^m \log_2\{L_{ij}(\Delta t)/L_{ij}(0)\} \qquad (3)$$

where the sum is over all m independent pairs of trial solutions, each with a random perturbation of the initial surface roughness. If we had infinite computer time we could run all possible initial conditions and so carry the average over all solution space. In practice we run a small number of trial problems with random initial conditions and take the result as an approximate estimate of the average. If we applied eq. (3) to a chaotic attractor and if we took care to pick only random initial points on the attractor then eq. (3) should be equivalent to eq. (1).

I have carried out numerical experiments modeling the Rayleigh Taylor instability using a two-dimensional incompressible Eulerian hydrodynamic code VFTS. The method of integrating the Navier-Stokes equations including the viscous terms is similar to that described in Kim & Moin [3], except that I have added Lagrange particles, and provision for body forces. The Eulerian method is 2^{nd} order accurate in both space and time, and the Poission equation for the effective pressure field is solved exactly at each time step using a cyclic reduction method.

For the Rayleigh-Taylor computations a Boussinesq forcing term is added that is valid for small Atwood numbers. The density field can be tracked with the Lagrange points and is used to compute the Boussinesq forcing term. With only two different densities it is not necessary to cover more than one of the regions with points, usually the one with the smaller area so as to maximize the resolution. The density to use in computing the Boussinesq forcing term is obtained from,

$$\rho_{ij}(t) = (\rho_p n_{ij}(t) + (n_o - n_{ij}(t))\rho_a) / n_o \qquad (4)$$

where ρ_p is the density of the liquid covered by the Lagrange net of points, ρ_a is the ambient liquid density, $n_{ij}(t)$ is the number of Lagrange points in Eulerian zone ij, and n_o is the initial number of points per zone.

A slightly different approach is to replace the Boussinesq term with a body force that is equal to a constant times the number of lagrange points in each Eulerian zone. In that case the density is everywhere the same but the body force is applied only over the region covered by the set of lagrange points. The two methods are computationally equivalent. The advantage of the body force is that the whole of the fluid can be accelerated relative to the rest frame yielding the partition of the work done on the fluid between the

kinetic energy of directed motion and the kinetic energy of the chaotic or turbulent motion.

Area is conserved by the Eulerian velocity field, in some cases to better than one part in 10^8 even after several thousand integration steps, due to the accuracy of the solution for the pressure field. As a result motion of the lagrange points also preserves area quite well, although further improvement could probably be obtained by using higher order methods to interpolate the velocity from the Eulerian mesh. One advantage of this method is that it can follow the evolution of the Rayleigh-Taylor instability well into the chaotic or turbulent regime.

The case I have experimented with consists of a thin, 3 cm, layer, imbedded in an ambient liquid of unit density. A constant body force acts on the layer, accelerating it and the rest of the liquid through the forces transmitted across the interface. The kinematic viscosity is constant and equal to .01 cm^2/s, ie., the physical values are for water. The code has periodic boundary conditions at horizontal and vertical intervals of 1.5 cm. A 60 x 60 Eulerian mesh was used, with 6480 Lagrange points covering the accelerated layer. The physical dimensions and constants of this case were chosen such that the computations should be able to accurately model viscous effects.

Some have reservations about the accuracy of combined lagrange particle-Eulerian methods. My experience is that they can maintain reasonably good accuracy in problems such as the Rayleigh Taylor instability provided the Eulerian zone size is kept in the viscous scale range, and provided the initial perturbation is not so small as to be quickly swamped by truncation error growth. In more quantitative terms it is desirable to keep the mesh size smaller than the wave length of the most rapidly growing disturbance predicted from linear analysis of the viscous case,

$$\Delta x < \lambda_m \approx 4\pi\ (\nu^2/Ag)^{1/3} \approx 4\pi\ (2\rho\nu^2/f)^{1/3} \qquad (5)$$

where f is the body force per unit volume, A is the Atwood number, g is the acceleration, ν is the kinematic viscosity, and λ_m is the wave length of the most rapidly growing perturbation.

There is always noise from round off and truncation error no matter what the computational method, and in Rayleigh Taylor unstable flows soon enough that noise will grow to a point that swamps all memory of the initial conditions. One can still estimate the average growth rate of the noise; it is just necessary to start with a big enough perturbation and keep the mesh size small enough to resolve the viscous scales of motion.

The results of the computations can be put in dimensionless form by normalizing the time by,

$$\tau = \sqrt{(\bar{\rho} d/f)} = \sqrt{(d/2Ag)} \qquad (6)$$

where d is the thickness of the layer.

I looked for a largest Lyapunov exponent like quantity by plotting the log(base 2) of the separation between pairs of solutions $L_{ij}(t)$. If there are N solutions, each for a different seed in the random number generator for the initial surface roughness, then there are N(N-1)/2 independent pairs of solutions. The separation between any two pairs of solutions has a large random component, but by including many cases on the same semilog plot, these random fluctuations can be averaged out leaving an approximation to the statistical limit. Six independent solutions is enough to give a good estimate when all fifteen possible pairs are plotted.

One example of the evolution of the instability and the breakup and rupture of the layer are shown in Fig. 1. Both the top and bottom surfaces of the layer have the same initial roughness, however only the

top surface goes unstable. The bottom surface remains stable and perturbations there decay in time because the computations include viscosity. All 6480 lagrange particles defining the layer are plotted. These are the coordinates used in Eq. (2) for computing the separation between two pairs of solutions.

The separation between any two pairs of solutions does appear to have a well defined statistical limiting curve. This can be seen in Fig. 2, where the $\log_2$ of the separation between the fifteen possible pairs of solutions for the case where the body force is 117.6 dynes/cm^3 are plotted. The dead space at the beginning of the runs (where $L_{ij}(t)$ is just equal to the initial separation due to a different seed in the initial roughness generator) is a numerical artifact; before anything can happen the layer has to move a sufficient distance for the initial roughness to show up as a perturbation on the underlying Eulerian mesh. Once the instability starts the separation between solutions $L_{ij}(t)$ grows rapidly - in these examples at a rate of about 125 bits/s - corresponding to the rate of growth derived from the linearized Rayleigh Taylor theory for the smallest wave length perturbation that can fit into the Eulerian mesh. This phase lasts only a very short time interval and results in an information growth of about 1.9 bits. After the initial transient, $\text{Log}_2[L(t)/L(0)]$ approaches a straight line asymptote with a slope of about 10 bits/s. Reference to Fig. 1 shows that most of the mixing leading to rupture of the layer takes place during this nonlinear asymptotic phase. When the time is put in dimensionless units by dividing by $\bar{\tau}$ from Eq. (6) then the asymptotic slope is 0.5 bits per unit time interval.

Similar results are obtained when the force is increased to 940.8 dynes/cm^3, corresponding to shortening the wave length of most rapid growth (in the viscous linear analysis) to 3 zones, or .075 cm. The time scale is shortened by a factor of $\sqrt{8}$ and the asymptotic slope increases to 28 bits/s; however in dimensionless units the slope remains 0.5 bits per unit time interval.

In fact, the behavior of all of the runs accumulated thus far is summarized by a single L(t) curve if the time is measured in units of τ. After adjusting the time origin to the take off point in Fig. 2

$$\mathrm{Log}_2[L(t)/L(0)] = 0.5t + 1.9\ [1 - e^{-3t}] \qquad (7)$$

seems to be a good estimate of the statistical limit. Eq. (7) only predicts the behavior in the sense that it approximates the most likely outcome for the rate of growth of information. Any individual numerical model run or experiment is likely to deviate significantly from Eq. (7) as can be seen from the variation in the runs shown in Fig. 2.

To show how Eq. (7) can be used to estimate the time a layer with given surface roughness will last before breaking up we apply it to the example in Fig. 1. In this case the initial position of the interface, measured in units of the thickness of the layer, is not very well defined, ie., the interface position is specified to only about 1 part in 12 or with about 3.6 bits of information. According to Eq. (7) approximately 3.6 bits of information ($\mathrm{Log}_2[L(t)/L(0)] = 3.6$) are generated by $t = 3.4$, or on converting to dimensional units by multiplying by τ, by roughly 0.17 seconds. Reference to Fig. 1 shows this is just about the time the layer begins to break up, after compensating for the .05 sec delay in starting. For every additional bit of information added in reducing the initial surface roughness or uncertainty in position the predictability time increases by 2τ or, in this case, by about 0.1 seconds.

To demonstrate that the chaotic behavior seen in Figs. 1 and 2 is not due to some numerical artifact I have included a case where the parameters are the same except that the initial surface perturbation is limited to a single cosine wave. Figure 3 shows a case with wave length 3 mm, and initial amplitude the same as the peak to peak limit in the white noise roughness cases. The wave length with the most

rapid rate of growth derived from viscous linear theory is 1.5 mm, same as for the cases in Fig. 2. Viscosity prevents singularites from developing, and the dimensions are small enough that one gets skirt formation along the sides of the bubbles instead of Kelvin-Helmholtz roll up . In the Boussinesq limit the Rayleigh-Taylor unstable upper surface should be symmetrical about its mid line until the amplitude grows to the point where the lower surface begins to affect the evolution. The computation should also maintain symmetry along the horizontal axis. Both these requirements are satisfied by the test computation.

CONCLUSION

Looked at from the viewpoint discussed above the Rayleigh-Taylor problem is similar to examples discussed in the nonlinear dynamics literature. I found, in the runs completed thus far, that the separation between any pair of solutions, after an initial transient, approaches an asymptotic rate of growth during the nonlinear stages of the evolution. On a semilog plot, except for individual statistical fluctuations, the curves of separation between any pair of solutions rapidly approach a single straight line asymptote. The constant rate of divergence in the nonlinear regime is more apparent when the statistical fluctuations are averaged out by plotting batches of pairs of runs together. Most of the mixing and rupture of the layer occurs during the asymptotic phase. In other words, during Youngs stage 2 - the nonlinear regime existing before fully developed turbulence, the flow seems to behave like a nonlinear chaotic system evolving on a low dimensional attractor. Worded in the terminology of nonlinear dynamics theory; there appears to be a statistically well defined rate of information production during this phase.

If such a largest Lyapunov exponent like quantity does exist it has several implications for the mix problem. For one it means there are inherent limits to the predictability of mix no matter how accurately the hydrodynamic equations are integrated. In particular it implies that Young's stage 2 is not much more predictable than the final turbulent stage. On the other hand, for giving something up you get something back; in this case the theory gives a statistical handle on the problem of estimating how rapidly mix will occur during the stage 2 phase. In these examples once the rate of information production has been determined its a simple calculation to estimate how long the layer will hang together, on average, given a specified amplitude of initial surface roughness.

References

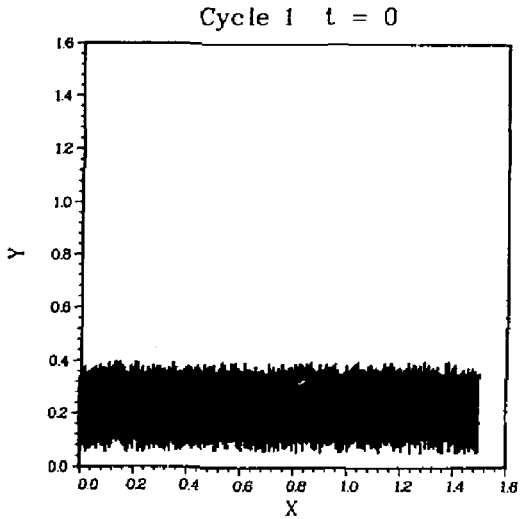
1. Youngs, D. L., Numerical Simulation of Turbulent Mixing by Rayleigh-Taylor Instability, Physica, 12D, 32-44 (1984).

2. Wolf, A., J. B. Swift, H. L. Swinney, and J. A. Vastano, Determining Lyapunov Exponents from a Time Series, Physica, 16D, 285-317 (1985).

3. Kim, J., and P. Moin, Application of a Fractional-Step Method to Incompressible Navier-Stokes Equations, J. Comp. Phys., 59, 308-323 (1985).

Figure 1

Typical evolution for the Rayleigh-Taylor mixing and rupture of the thin layers. The dimensions of the 60 x 60 computational grid are 1.5 cm by 1.5 cm with periodic boundary conditions at the edges. Thickness of the thin layer is 3 mm, mean density of the liquid is 1 g/cm^3, kinematic viscosity is .01 cm^2/s, and the body force (twice the Atwood number times the acceleration times the average density) applied to the thin layers is 117.6 $dynes/cm^3$. The surfaces of the layer are perturbed by a white noise roughness distribution with maximum amplitude .05 cm. The most rapidly growing wave length derived from linear analysis of the viscous Rayleigh-Taylor instability is .15 cm, or half the thickness of the layer. The layer appears to rupture well before Young's stage 3 (the fully developed turbulence regime) is reached. The results can be scaled to a range of other parameter values by dimensional analysis.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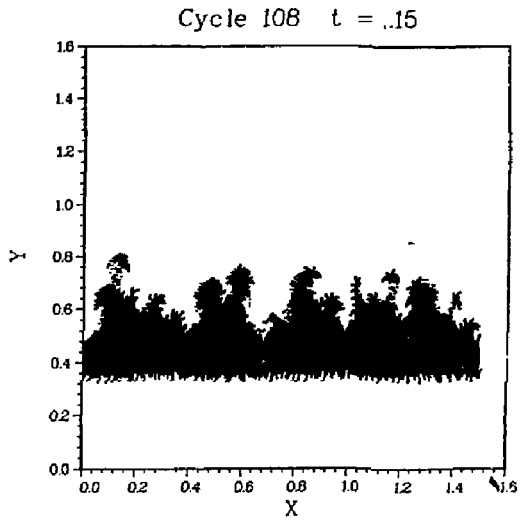
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X
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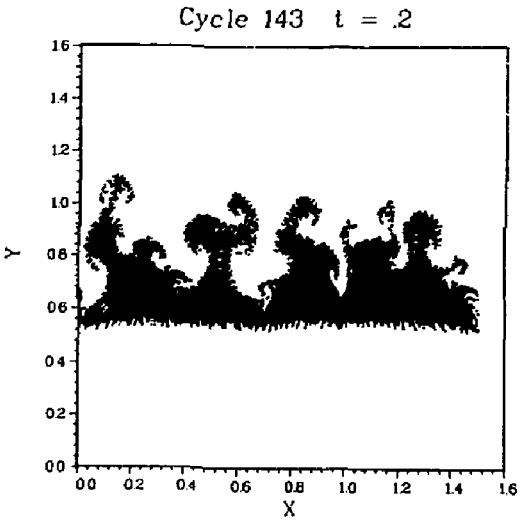
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X
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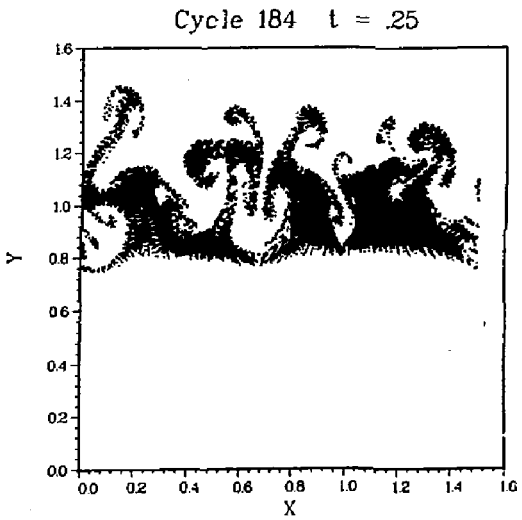
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X
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Figure 2

The log (base 2) of the separation L(t) between pairs of solutions normalized by the initial separation plotted versus time. L(t) is determined from the time history of Lagrange particles embedded in the layer and saved from each 2D solution of the Navier-Stokes equations. It is equal to the square root of the sum over all 6480 labeled particles of the squares of the differences in coordinates of each pair of particles with the same initial coordinates (before adding roughening) taken from a given pair of 2D solutions. Each 2D solution is different because each run starts with a different seed in the random number generator for the initial white noise roughening of the layer surfaces. The dead interval at the beginning results from the time it takes for the layer to translate approximately one zone starting from rest, ie., nothing happens on scales less than can be resolved by the mesh. The maximum roughness variation is .05 cm or two zones, swamping any perturbations due to spatial truncation effects.

Curves for the 15 different pairings possible from 6 different solutions are included on one plot to give a better idea of the underlying statistics. The initial slope of the plot is approximately 125 bits/s. After the initial steep rise there is a rapid approach to an asymptotic rate of growth of approximately 10 bits/s. Reference to Figure 1 shows that most of the evolution of the mix - before rupture of the layer - occurs during this nonlinear asymptotic phase. If the asymptotic state represents evolution along a low dimensional attractor, then the slope - 10 bits/s - should be the approximate value of the largest Lyapunov exponent.

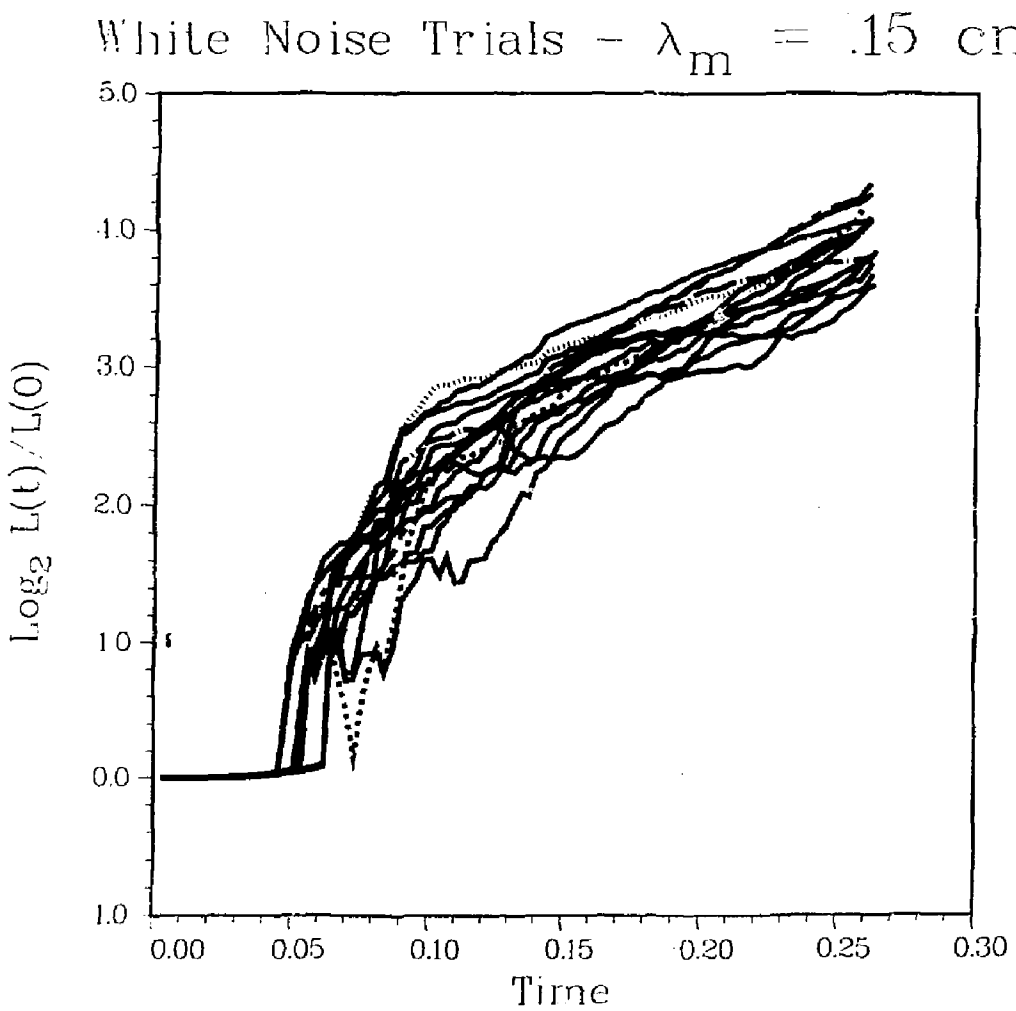
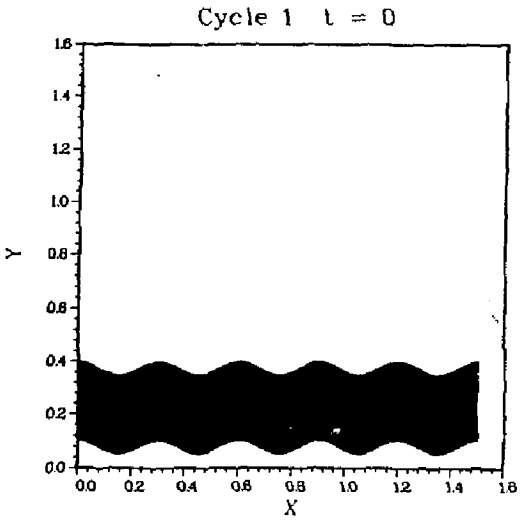

White Noise Trials – λ_m = .15 cm
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
Log_2 L(t)/L(0)
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Time

Figure 3

Demonstration that the chaotic evolution seen in the random surface roughness trials is not due to numerical effects. Same parameters as in the roughness cases, with same amplitude of initial surface perturbation, but single wave length cosine perturbation of the surface.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X
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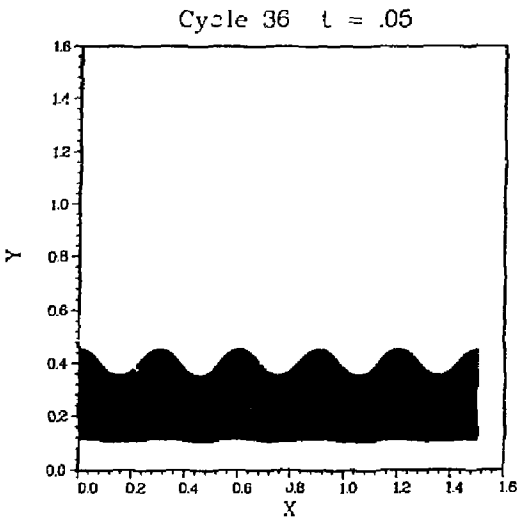
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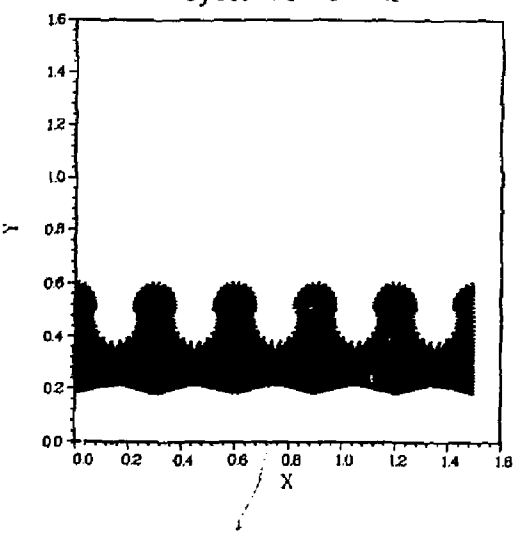
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X
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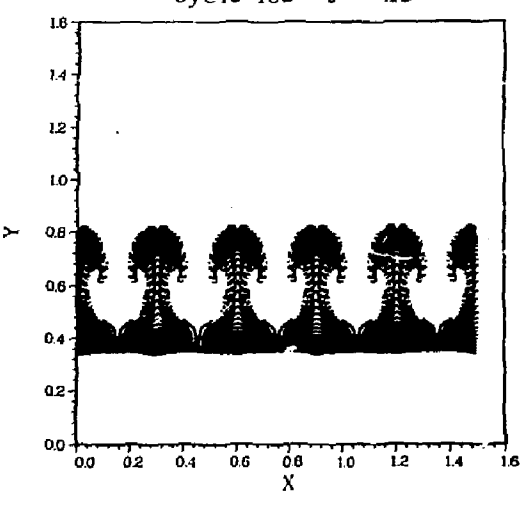
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Y
X
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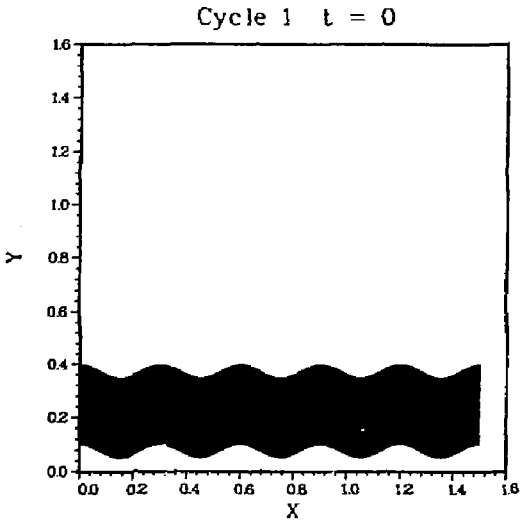
Cycle 1 t = 0
Y
X
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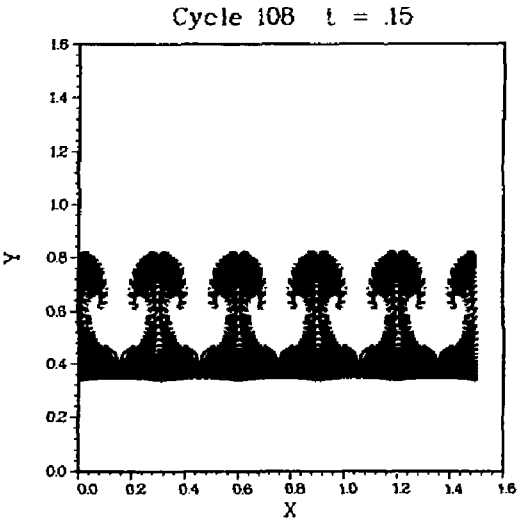
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6


Cycle 108 t = .15
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X
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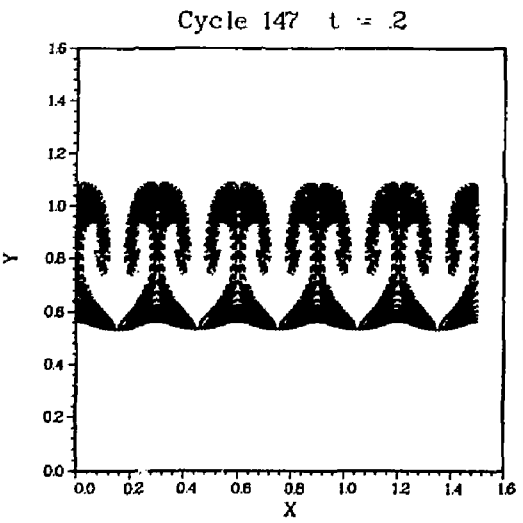
0.8
1.0
1.2
1.4
1.6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X
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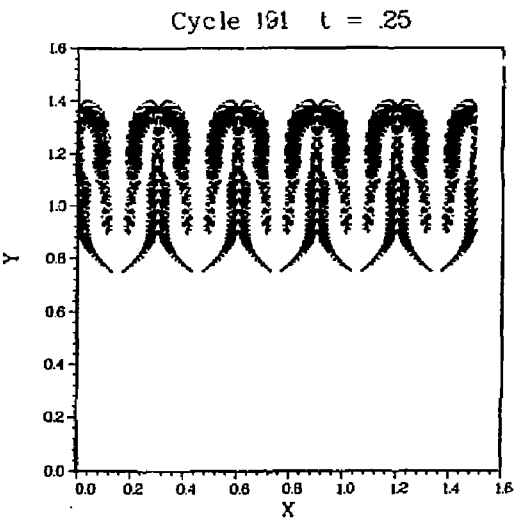
1.4
1.6


Cycle 191 t = .25
Y
X
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0.4
0.6
0.8
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1.2
1.4
1.6